Harmonically trapped dipolar fermions in a two-dimensional square lattice

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We consider dipolar fermions in a two-dimensional square lattice and a harmonic trapping potential. The anisotropy of the dipolar interaction combined with the lattice leads to transitions between phases with density order of different symmetries. We show that the attractive part of the dipolar interaction results in a superfluid phase which is suppressed by density order. The trapping potential is demonstrated to make the different phases co-exist, forming ring and island structures. The phases with density and superfluid order can overlap forming regions with supersolid order.

The trapping of dipolar atoms and molecules is a promising new research field. The anisotropy of the dipole interaction offers unique opportunities for exploring novel few-body [1, 2] and many-body quantum systems [3, 4]. Experimentally, one has realized Bose-Einstein condensates of ^{52}Cr atoms [5, 6] and ^{164}Dy atoms [7] with large magnetic dipole moments, as well as gases close to quantum degeneracy of ^{40}K^{87}Rb molecules with an electric dipole moment [8]. Furthermore, the first experimental steps toward realizing dipolar molecules in an optical lattice have recently been reported [9, 10]. The lattice makes the physics very rich: Density ordered phases with a complicated unit cell [11], liquid crystal phases [12], and a supersolid phase [13] have been predicted to exist for fermionic dipoles in a 2D lattice with dipole moments perpendicular to the lattice plane, and tilting the dipoles towards the lattice plane leads to bond-solid order and p-wave superfluidity at half-filling [14].

We consider fermionic dipoles in a 2D square lattice at zero temperature. A harmonic potential, which is always present in trapped atomic/molecular systems, is included exactly, since the characteristic lengths of the ordered phases can be comparable to the system size for experimentally realistic systems. This means that one cannot simply resort to the local density approximation. A main purpose of the present paper is to study the rich physics coming from the interplay between the anisotropic dipole interaction, the optical lattice, and the inhomogeneity induced by the trapping potential. For experimentally realistic systems, we demonstrate the existence of competing phases with density order of checker-board or stripe symmetry, and superfluid order. Due to the trapping potential, these phases can co-exist and sometimes even spatially overlap leading to regions with supersolid order.

Basic formalism The fermions have a mass m and a dipole moment $\mathbf{d}$ which is aligned by an external field forming the angle θ_P with the z-axis perpendicular to the lattice (xy) plane and the azimuthal angle ϕ_P with respect to one of the lattice vectors parallel to the x-axis, see Fig. 1. In the lowest band approximation, this system is described by the extended Hubbard model with the Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}$ where

$$\hat{H}_0 = -t\sum_{\langle ij\rangle}\left(\hat{c}_i^\dagger \hat{c}_j + h.c.\right) + \sum_i \left(\frac{1}{2}m\omega^2 r_i^2 - \mu\right)\hat{n}_i \quad (1)$$

and

$$\hat{V} = \frac{1}{2}\sum_{i\neq j} V_D(\mathbf{r}_{ij})\hat{n}_i\hat{n}_j \quad (2)$$

with $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$. Here, $\hat{c}_i$ removes a dipole at site i with position $\mathbf{r}_i$, $\hat{n}_i = \hat{c}_i^\dagger \hat{c}_i$, μ is the chemical potential, t is the hopping matrix element between nearest neighbor sites $\langle ij\rangle$, and $i \neq j$ since we are considering identical fermions. The trapping frequency is ω and the interaction between two dipoles separated by $\mathbf{r}$ is

$$\begin{aligned} V_D(\mathbf{r}) &= \frac{D^2}{r^3}\left[1 - 3\cos^2(\theta_{\rm rd})\right] \\ &= \frac{D^2}{r^3}\left[1 - 3\cos^2(\phi_P - \phi)\sin^2(\theta_P)\right] \end{aligned} \quad (3)$$

with $D^2 = d^2/4\pi\epsilon_0$ for electric dipoles and $\theta_{\rm rd}$ the angle between $\mathbf{d}$ and $\mathbf{r} = r(\cos\phi, \sin\phi, 0)$, see Fig. 1.

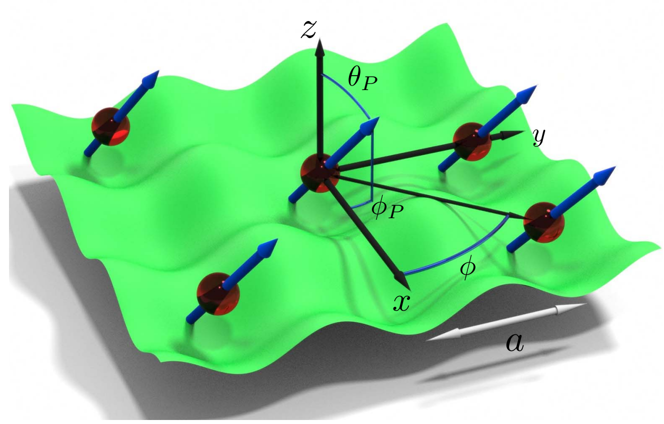

FIG. 1: (color on-line) We consider dipoles in a square 2D lattice in the xy-plane. The dipoles are aligned forming an angle θ_P with the z-axis and the azimuthal angle ϕ_P with the x-axis which is parallel to one of the lattice vectors.

Since the dipolar interaction (3) has both attractive and repulsive regions, the system exhibits both pairing and density instabilities depending on (θ_P, ϕ_P). To model this complex behavior, we decouple the interaction $\hat{V}$ using the mean-field approximation which yields

$$\hat{V}_{\rm MF} = \sum_{i\neq j} V_D(\mathbf{r}_{ij}) \left(\langle \hat{n}_j \rangle \hat{n}_i - \frac{1}{2} \langle \hat{n}_j \rangle \langle \hat{n}_i \rangle \right)$$
$$+ \sum_{i\neq j} \frac{V_D(\mathbf{r}_{ij})}{2} \left(\langle \hat{c}_j \hat{c}_i \rangle \, \hat{c}_i^\dagger \hat{c}_j^\dagger + h.c. - |\, \langle \hat{c}_j \hat{c}_i \rangle \,|^2 \right) \quad (4)$$

where $\langle \hat{c}_j \hat{c}_i \rangle$ is the pairing order parameter. Even though fluctuations are important in 2D, we expect mean-field theory to capture the existence and competition between different ordered phases at $T = 0$. Indeed, mean-field theory is widely used in the high-T_c community to describe the competition between e.g. anti-ferromagnetic and superfluid ordering [15]. We have not included the Fock term in (4), since one dipole interacts with many others making the problem similar to a high dimensional one, for which the Hartree term dominates [16]. The Fock term has recently been shown to lead to bond-solid order phases at half-filling [14].

The mean-field Hamiltonian $\hat{H}_0 + \hat{V}_{\rm MF}$ is diagonalized by the Bogoliubov transformation $\hat{c}_i = \sum_{E_\eta > 0} (u_\eta^i \hat{\gamma}_\eta + v_\eta^{i*} \hat{\gamma}_\eta^\dagger)$ where γ_η are fermionic operators annihilating a quasi-particle with energy E_η. The wave functions u_η^i and v_η^i satisfy the Bogoliubov-de Gennes equations

$$\sum_j \begin{pmatrix} L_{ij} & \Delta_{ij} \\ \Delta_{ji}^* & -L_{ij} \end{pmatrix} \begin{pmatrix} u_\eta^j \\ v_\eta^j \end{pmatrix} = E_\eta \begin{pmatrix} u_\eta^i \\ v_\eta^i \end{pmatrix}, \quad (5)$$

with $\Delta_{ij} = V_D(\mathbf{r}_{ij}) \langle \hat{c}_j \hat{c}_i \rangle$ and

$$L_{ij} = -t\delta_{\langle ij \rangle} + (\sum_k V_D(\mathbf{r}_{ik}) \langle n_k \rangle + \frac{m}{2} \omega^2 r_i^2 - \mu) \delta_{ij}. \quad (6)$$

Here δ_{ij} and $\delta_{\langle ij \rangle}$ are the Kronecker delta functions connecting on-site and nearest neighbor sites, respectively. Self-consistency is obtained iteratively through the usual relations: $\langle \hat{n}_i \rangle = \sum_{E_\eta > 0} |v_\eta^i|^2$ and $\langle \hat{c}_i \hat{c}_j \rangle = \sum_{E_\eta > 0} u_\eta^i v_\eta^{j*}$.
No trapping potential Consider first a system with no trapping potential. We plot in Fig. 2 the ground state as a function of the dipolar angles (θ_P, ϕ_P) in the limit of strong interactions $g/t = 16$ with $g = D^2/a^3$ where a is the lattice constant. The filling fraction is $f = N^{-1} \sum_i \langle \hat{n}_i \rangle = 1/2$ with N the number of lattice sites. We consider two possible ground states: One with a checker-board density order and one with a striped density order. The $+$ symbols and the $\times$ symbols indicate when mean-field theory on a 26×26 lattice predicts the checker-board phase and the striped phase to have the lowest energy, respectively. In order to take into account the long-range nature of the dipolar interaction we have calculated the Hartree term by duplicating the 26×26 lattice so that it constitutes a lattice of $9 \cdot 26 \times 9 \cdot 26$ sites. For small θ_P, the checker-board phase is favored whereas for larger θ_P a phase with stripes along the x-direction has the lowest energy. This is easily understood for $\phi_P = 0$, where the dipoles are aligned head-to-tail in this phase which clearly minimizes the interaction energy. When $\phi_P > 0$, the alignment is not perfect by stripe formation along the x-axis, but the interaction energy is still minimized although it requires larger tilting angles θ_P as expected. This is illustrated further by the dashed line separating the checker-board phase from the striped phase, which is a result of comparing the classical interaction energy in the two phases. The good agreement

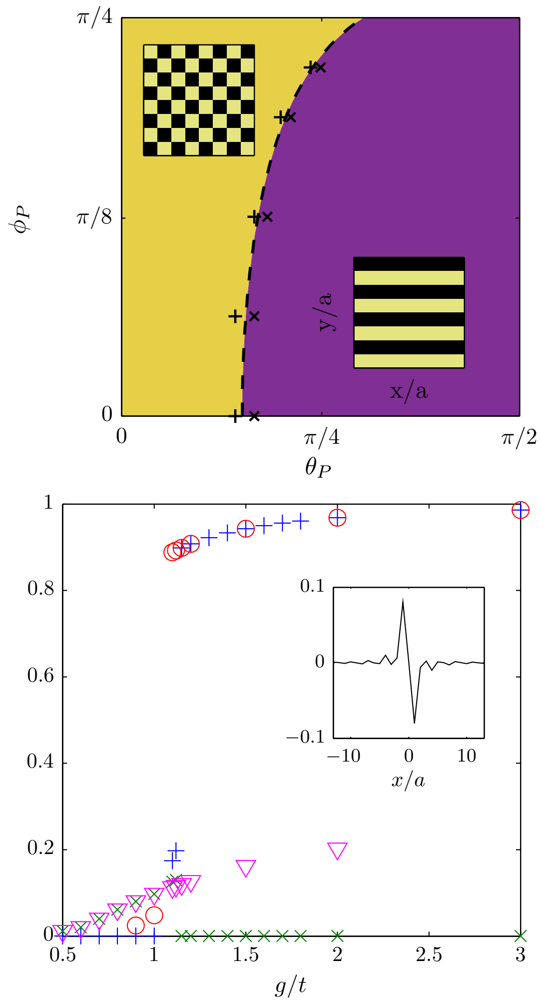

FIG. 2: (color on-line) Top: The phase-diagram for an untrapped system for strong coupling $g/t = 16$ and half-filling. The dashed line shows the boundary between the checker-board and the striped phase. Bottom: The nearest neighbor pairing $|\langle \hat{c}_{i+\hat{x}} \hat{c}_i \rangle|$ ($\times$'s) and stripe order $|\langle \hat{n}_i - \hat{n}_{i+\hat{y}} \rangle|$ ($+$'s) as a function of g/t with $(\theta_P, \phi_P) = (\pi/2, 0)$. The $\circ$'s show $|\langle n_i - n_{i+\hat{y}} \rangle|$ when we take the gap to be zero. The $\triangledown$'s show $|\langle \hat{c}_{i+\hat{x}} \hat{c}_i \rangle|$ when the density is taken to be homogeneous. The inset shows a cut of $\langle \hat{c}_{i+\hat{x}} \hat{c}_i \rangle$ along the x-axis when $g/t = 0.9$.

between the numerics and this calculation demonstrates that for strong coupling $g/t \gg 1$ the kinetic energy can be neglected, and the problem becomes classical.

When $\theta_P \geq \arcsin(1/\sqrt{3}) \approx 0.2\pi$, the interaction has attractive regions, and we now examine the competition between the resulting pairing instability and the instability towards density order. In Fig. 2, we plot as $\times$'s the largest value of the nearest neighbor pairing $|\langle \hat{c}_{i+\hat{x}}\hat{c}_i\rangle|$ as a function of the coupling strength g/t with $\hat{x}$ a unit vector along the x-direction. We have chosen $(\theta_P, \phi_P) = (\pi/2, 0)$ and $f = 1/3$. The calculations are performed on a 27×27 lattice. For weak coupling, the ground state is a superfluid. The cross section along the x-axis of the pair wave function $\langle \hat{c}_j \hat{c}_i\rangle$ with $\mathbf{r}_i = (0, 0)$ plotted in the inset, illustrates that it is odd under inversion as for the homogeneous case [17, 18]. For simplicity, we refer to this as p-wave symmetry in the following, even though the pair wave function in general contains higher odd components of angular momenta. For stronger coupling, the pairing vanishes as the striped phase emerges. The stripe order defined as $\langle \hat{n}_i - \hat{n}_{i+\hat{y}}\rangle$, with $\hat{y}$ a unit vector along the y-direction so that $\langle \hat{n}_i\rangle$ and $\langle \hat{n}_{i+\hat{y}}\rangle$ give the densities for a site in the stripe and next to the stripe respectively, is plotted as $+$'s in Fig. 2. We also plot as $\circ$'s the stripe order parameter when pairing is not included in the calculation, and as ∇'s the pairing order parameter when the stripe formation is not included. This demonstrate that the stripe order is insensitive to pairing since the critical coupling strength for the formation of stripes essentially does not change when pairing is included. The pairing on the other hand does not vanish with increasing coupling if the stripes are suppressed. We therefore conclude that it is the pairing which is suppressed by the stripe formation and not the other way around.

More complicated density order with larger unit cells can appear for untrapped systems, as has recently been demonstrated for $\theta_P = 0$ [11]. Here, we focus on the experimentally most relevant orders with the smallest unit cell, since the trapping potential will complicate the observation of orders with a large unit cells.

Trapped case We now examine the interplay between the harmonic trapping potential and the competition between density and pairing instabilities.

Angle $\theta_P = 0$ Consider first the case when the dipolar orientation is perpendicular to the lattice so that the interaction is purely repulsive. Figure 3 shows the density profile for trapped dipoles with $\tilde{\omega} = \omega a\sqrt{m/t} = 0.24$ which is a relatively weak trapping potential so that there are regions with phases resembling those for the case with no trapping potential. For $g/t = 0.5$ and 144 particles, there is no density order whereas for stronger coupling $g/t = 1$ and 207 particles, the system exhibits a checker-board density profile in the center of the trap. In this region, $f \simeq 1/2$ which is optimal for the checker-board phase [11]. The checker-board phase is surrounded by a normal phase with a lower density. Experimentally, similar shell structures have been observed for atoms with a short range interaction [19].

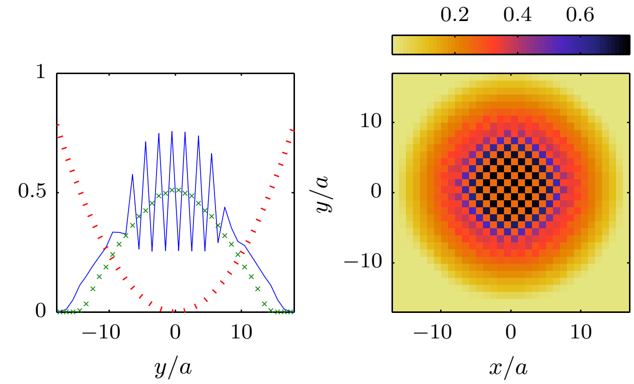

FIG. 3: (color on-line) Left: The density profile through the center of the trap. The blue solid line is for $g/t = 1$ and 207 particles trapped and the green crosses are for $g/t = 0.5$ and 144 particles trapped. The red dotted line indicates the trapping potential in units of 2.5t with $\tilde{\omega} = 0.24$. Right: 2D plot of the density in the lattice plane for the $g/t = 1$ case.

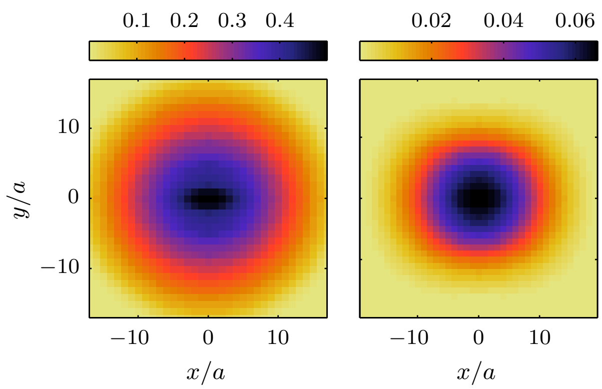

FIG. 4: (color on-line) Left: The particle density for 205 dipoles with $\theta_P = \pi/2$, $g/t = 0.85$, and $\tilde{\omega} = 0.11$. Right: The nearest neighbor pairing $(|\langle \hat{c}_{i+\hat{x}}\hat{c}_i\rangle| + |\langle \hat{c}_{i-\hat{x}}\hat{c}_i\rangle|)/2$.

Angles $(\theta_P, \phi_P) = (\pi/2, 0)$ Consider next the case when the dipoles are aligned in the plane along the x-axis ($\phi_P = 0$). There is then a competition between density and pairing order. In Fig. 4, we plot the density and the nearest neighbor pairing $(|\langle \hat{c}_{i+\hat{x}}\hat{c}_i\rangle| + |\langle \hat{c}_{i-\hat{x}}\hat{c}_i\rangle|)/2$ (symmetrized to reduce trap effects) for $g/t = 0.85$, $\tilde{w} = 0.11$ and 205 dipoles trapped in a 39×39 lattice. For this set of parameters, there is no density order since the density is low and the interaction weak. This results in p-wave pairing throughout most of the cloud. The cloud profile is slightly elongated in the x-direction due to the anisotropy of the dipolar interaction in analogy with what has been observed for dipolar condensates [4].

Figure 5 depicts the density and the nearest neighbor pairing for a stronger coupling strength $g/t = 1$ with $\tilde{w} = 0.11$ and 180 dipoles trapped on a 39×39 lat-

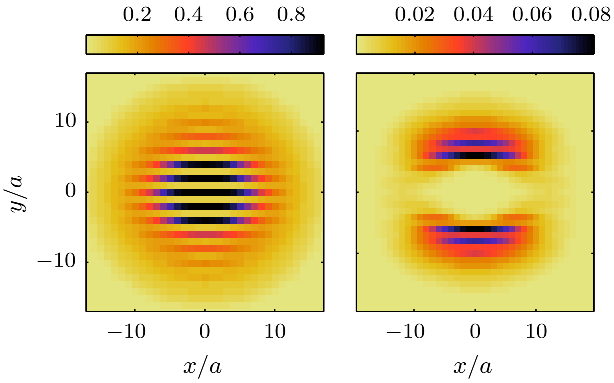

FIG. 5: (color on-line) Left: The density profile for 180 dipoles with $\theta_P = \pi/2$, $g/t = 1$, and $\tilde{\omega} = 0.11$. Right: The nearest neighbor pairing $(|\langle \hat{c}_{i+\hat{x}} \hat{c}_i \rangle| + |\langle \hat{c}_{i-\hat{x}} \hat{c}_i \rangle|)/2$.

tice. There is a pronounced stripe order in the center of the trap with an average filling fraction $f \simeq 1/2$ which squeezes the pairing away from the center into two islands centered at $x = 0$. This intriguing island structure is a consequence of the anisotropy of the interaction. Since the interaction is attractive when the dipoles are aligned head-to-tail (x-direction) and repulsive when they are side-by-side (y-direction), the average interaction for a given radius is attractive in the regions close to the y-axis whereas it is repulsive in the regions close to the x-axis. Thus, pairing can exist in the islands around $x = 0$ away from the center where stripe order dominates, whereas it is suppressed in the regions around $y = 0$. These islands of pairing should be compared with the ring structures predicted for a two-component trapped fermi gas with a short range isotropic repulsive interaction where anti-ferromagnetic order competes with d-wave pairing [20]. Remarkably, the stripe order is not completely suppressed in the two islands of pairing. The pairing in fact oscillates *in-phase* with the stripe order. This indicates that the trapping potential induces regions of pairing co-existing with density order as in a supersolid – a phase which has been subject to intense investigations since its theoretical prediction long ago [21–25].

The lattices considered here have experimentally realistic sizes, and with electric dipole moments up to several Debye for the experimentally relevant KRb, RbCs, and LiCs molecules [8, 26–28], one can easily reach the strong-coupling regime with $g/t \gg 1$ using typical values for an optical lattice. The density ordering can be observed directly by in-situ imaging [29] or by time-of-flight experiments which also can detect pairing correlations [20, 30].

In conclusion, we have shown that dipolar fermions at $T = 0$ in a 2D square lattice exhibit phases of density order with different symmetries as well as a p-wave superfluid phase. The system is unstable towards pairing when the interaction has attractive channels. However, any superfluidity is suppressed if there is an instability towards stripe formation such as in regions with a density close to half filling. The trapping potential leads to an inhomogeneous filling fraction which results in the co-existence of several phases. These phases can overlap resulting in the presence of regions with supersolid order.

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